

Electronic Supplementary Information (ESI) available for:

**Theoretical Study on Novel Alkaline Earth-Based Excess Electron  
Compounds: Unique Alkalides with Considerable Nonlinear Optical  
Responses**

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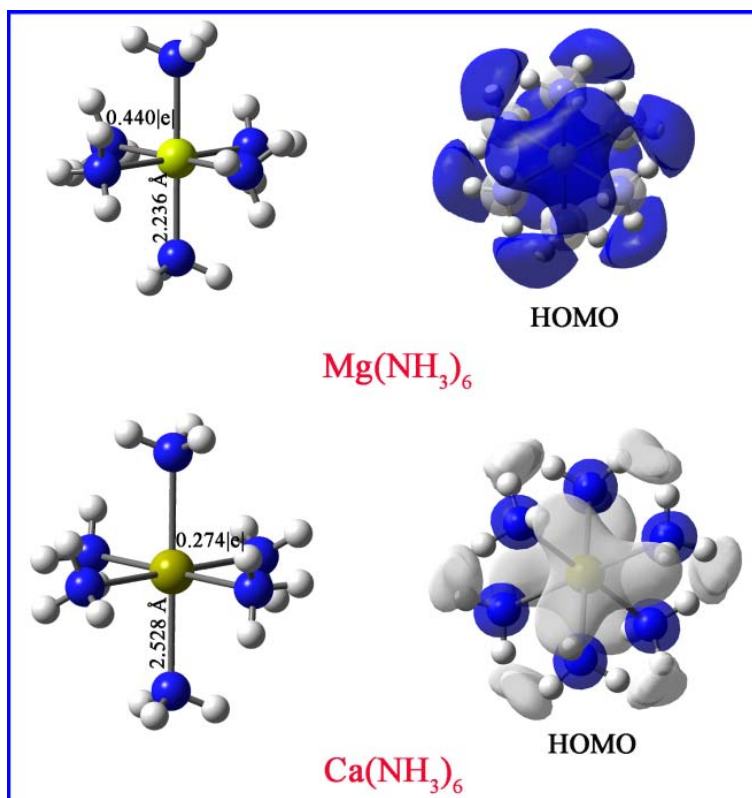
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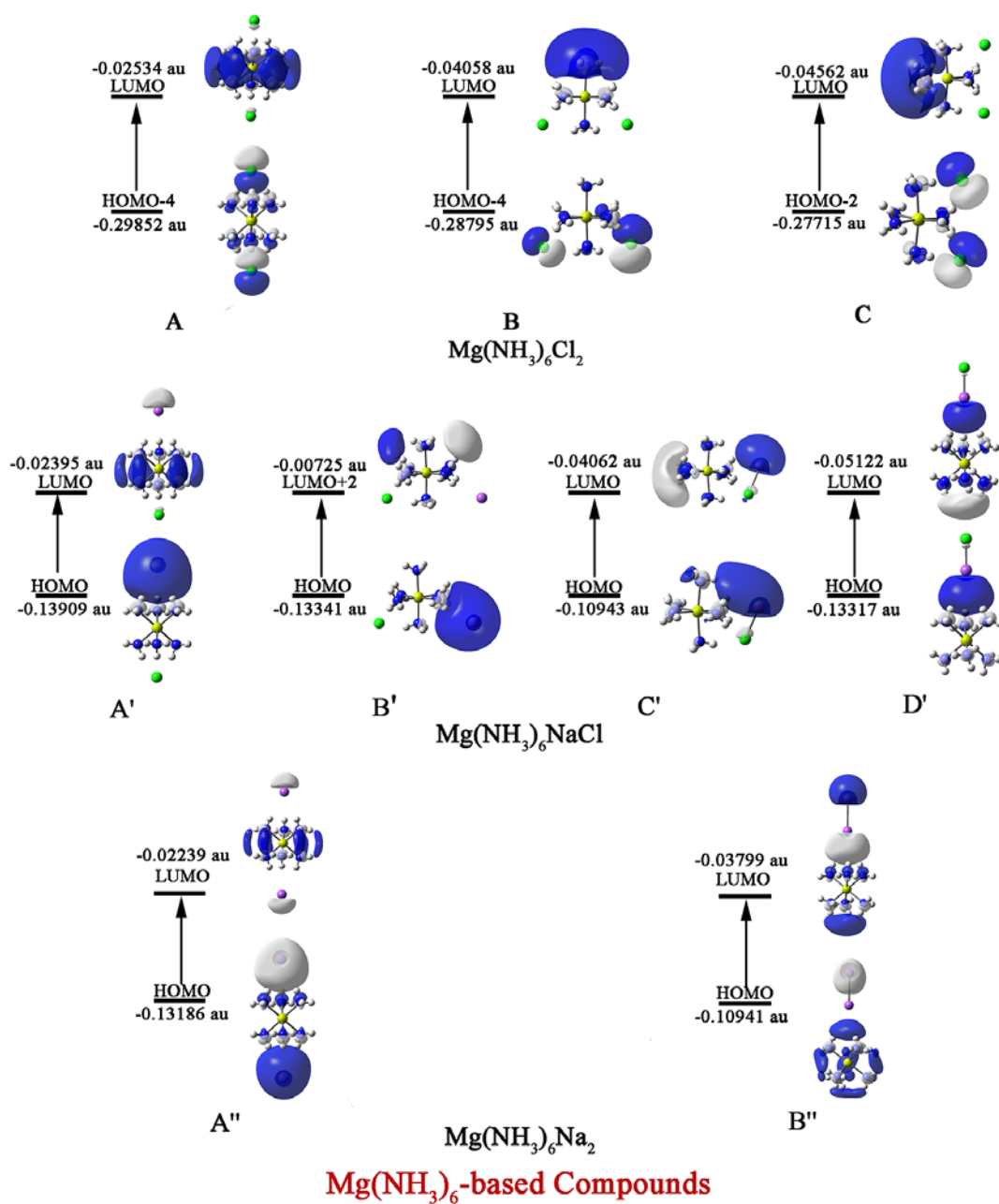
E-mail address: [liyingedu@jlu.edu.cn](mailto:liyingedu@jlu.edu.cn)

## 1. Figures and Table

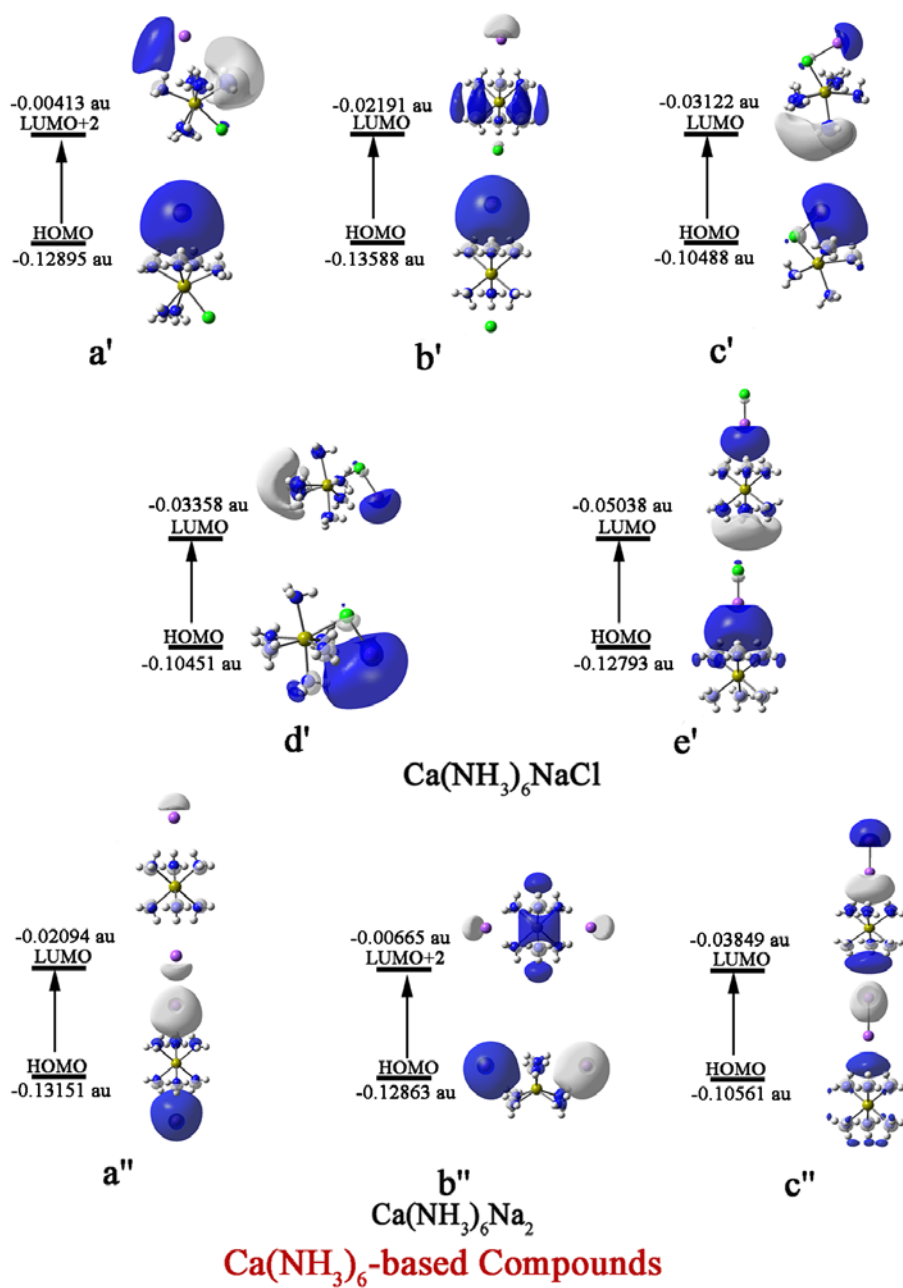
**Fig. S1.** Structures and HOMOs of isolated  $\text{Mg}(\text{NH}_3)_6$  and  $\text{Ca}(\text{NH}_3)_6$  amines.



**Fig. S2.** Crucial transitions of the  $\text{Mg}(\text{NH}_3)_6$ -based compounds.



**Fig. S3.** Crucial transitions of the  $\text{Ca}(\text{NH}_3)_6$ -based compounds.



**Table S1** Selected dissociation channels and ZPVE-corrected dissociation energies ( $D_e$ ) for the  $\text{Mg}(\text{NH}_3)_6^-$  and  $\text{Ca}(\text{NH}_3)_6^-$ -based complexes at the CAM-B3LYP/6-311++G(d, p) level.

Complex	Isomers	Dissociation channels	$D_e/\text{kcal}\cdot\text{mol}^{-1}$
$\text{Mg}(\text{NH}_3)_6\text{Cl}_2$	<b>A</b>	$\text{Mg}(\text{NH}_3)_6\text{Cl}_2 \rightarrow \text{Mg}(\text{NH}_3)_6 + 2\text{Cl}$	224.9
		$\text{Mg}(\text{NH}_3)_6\text{Cl}_2 \rightarrow \text{Mg} + 6\text{NH}_3 + 2\text{Cl}$	258.2
	<b>B</b>	$\text{Mg}(\text{NH}_3)_6\text{Cl}_2 \rightarrow \text{Mg}(\text{NH}_3)_6 + 2\text{Cl}$	217.8
		$\text{Mg}(\text{NH}_3)_6\text{Cl}_2 \rightarrow \text{Mg} + 6\text{NH}_3 + 2\text{Cl}$	251.1
	<b>C</b>	$\text{Mg}(\text{NH}_3)_6\text{Cl}_2 \rightarrow \text{Mg}(\text{NH}_3)_6 + 2\text{Cl}$	211.6
		$\text{Mg}(\text{NH}_3)_6\text{Cl}_2 \rightarrow \text{Mg} + 6\text{NH}_3 + 2\text{Cl}$	244.9
$\text{Mg}(\text{NH}_3)_6\text{NaCl}$	<b>A'</b>	$\text{Mg}(\text{NH}_3)_6\text{NaCl} \rightarrow \text{Mg}(\text{NH}_3)_6 + \text{Na} + \text{Cl}$	128.5
		$\text{Mg}(\text{NH}_3)_6\text{NaCl} \rightarrow \text{Mg} + 6\text{NH}_3 + \text{Na} + \text{Cl}$	161.8
	<b>B'</b>	$\text{Mg}(\text{NH}_3)_6\text{NaCl} \rightarrow \text{Mg}(\text{NH}_3)_6 + \text{Na} + \text{Cl}$	123.7
		$\text{Mg}(\text{NH}_3)_6\text{NaCl} \rightarrow \text{Mg} + 6\text{NH}_3 + \text{Na} + \text{Cl}$	157.0
	<b>C'</b>	$\text{Mg}(\text{NH}_3)_6\text{NaCl} \rightarrow \text{Mg}(\text{NH}_3)_6 + \text{Na} + \text{Cl}$	116.1
		$\text{Mg}(\text{NH}_3)_6\text{NaCl} \rightarrow \text{Mg}(\text{NH}_3)_6 + \text{NaCl}$	23.0
	<b>D'</b>	$\text{Mg}(\text{NH}_3)_6\text{NaCl} \rightarrow \text{Mg} + 6\text{NH}_3 + \text{Na} + \text{Cl}$	149.4
		$\text{Mg}(\text{NH}_3)_6\text{NaCl} \rightarrow \text{Mg}(\text{NH}_3)_6 + \text{Na} + \text{Cl}$	102.4
		$\text{Mg}(\text{NH}_3)_6\text{NaCl} \rightarrow \text{Mg}(\text{NH}_3)_6 + \text{NaCl}$	9.3
		$\text{Mg}(\text{NH}_3)_6\text{NaCl} \rightarrow \text{Mg} + 6\text{NH}_3 + \text{Na} + \text{Cl}$	135.7
$\text{Mg}(\text{NH}_3)_6\text{Na}_2$	<b>A''</b>	$\text{Mg}(\text{NH}_3)_6\text{Na}_2 \rightarrow \text{Mg}(\text{NH}_3)_6 + 2\text{Na}$	31.5
		$\text{Mg}(\text{NH}_3)_6\text{Na}_2 \rightarrow \text{Mg} + 6\text{NH}_3 + 2\text{Na}$	64.8
	<b>B''</b>	$\text{Mg}(\text{NH}_3)_6\text{Na}_2 \rightarrow \text{Mg}(\text{NH}_3)_6 + 2\text{Na}$	18.8
		$\text{Mg}(\text{NH}_3)_6\text{Na}_2 \rightarrow \text{Mg}(\text{NH}_3)_6 + \text{Na}_2$	2.9
		$\text{Mg}(\text{NH}_3)_6\text{Na}_2 \rightarrow \text{Mg} + 6\text{NH}_3 + 2\text{Na}$	52.1
$\text{Ca}(\text{NH}_3)_6\text{NaCl}$	<b>a'</b>	$\text{Ca}(\text{NH}_3)_6\text{NaCl} \rightarrow \text{Ca}(\text{NH}_3)_6 + \text{Na} + \text{Cl}$	134.0
		$\text{Ca}(\text{NH}_3)_6\text{NaCl} \rightarrow \text{Ca} + 6\text{NH}_3 + \text{Na} + \text{Cl}$	197.2
	<b>b'</b>	$\text{Ca}(\text{NH}_3)_6\text{NaCl} \rightarrow \text{Ca}(\text{NH}_3)_6 + \text{Na} + \text{Cl}$	130.7
		$\text{Ca}(\text{NH}_3)_6\text{NaCl} \rightarrow \text{Ca} + 6\text{NH}_3 + \text{Na} + \text{Cl}$	193.9
	<b>c'</b>	$\text{Ca}(\text{NH}_3)_6\text{NaCl} \rightarrow \text{Ca}(\text{NH}_3)_6 + \text{Na} + \text{Cl}$	123.8
		$\text{Ca}(\text{NH}_3)_6\text{NaCl} \rightarrow \text{Ca}(\text{NH}_3)_6 + \text{NaCl}$	30.7
	<b>d'</b>	$\text{Ca}(\text{NH}_3)_6\text{NaCl} \rightarrow \text{Ca} + 6\text{NH}_3 + \text{Na} + \text{Cl}$	187.0
		$\text{Ca}(\text{NH}_3)_6\text{NaCl} \rightarrow \text{Ca}(\text{NH}_3)_6 + \text{Na} + \text{Cl}$	122.3
		$\text{Ca}(\text{NH}_3)_6\text{NaCl} \rightarrow \text{Ca}(\text{NH}_3)_6 + \text{NaCl}$	29.23
		$\text{Ca}(\text{NH}_3)_6\text{NaCl} \rightarrow \text{Ca} + 6\text{NH}_3 + \text{Na} + \text{Cl}$	185.5
	<b>e'</b>	$\text{Ca}(\text{NH}_3)_6\text{NaCl} \rightarrow \text{Ca}(\text{NH}_3)_6 + \text{Na} + \text{Cl}$	102.8
		$\text{Ca}(\text{NH}_3)_6\text{NaCl} \rightarrow \text{Ca}(\text{NH}_3)_6 + \text{NaCl}$	9.7
		$\text{Ca}(\text{NH}_3)_6\text{NaCl} \rightarrow \text{Ca} + 6\text{NH}_3 + \text{Na} + \text{Cl}$	165.9
$\text{Ca}(\text{NH}_3)_6\text{Na}_2$	<b>a''</b>	$\text{Ca}(\text{NH}_3)_6\text{Na}_2 \rightarrow \text{Ca}(\text{NH}_3)_6 + 2\text{Na}$	33.2
		$\text{Ca}(\text{NH}_3)_6\text{Na}_2 \rightarrow \text{Ca} + 6\text{NH}_3 + 2\text{Na}$	96.4
	<b>b''</b>	$\text{Ca}(\text{NH}_3)_6\text{Na}_2 \rightarrow \text{Ca}(\text{NH}_3)_6 + 2\text{Na}$	30.8
		$\text{Ca}(\text{NH}_3)_6\text{Na}_2 \rightarrow \text{Ca} + 6\text{NH}_3 + 2\text{Na}$	94.0
	<b>c''</b>	$\text{Ca}(\text{NH}_3)_6\text{Na}_2 \rightarrow \text{Ca}(\text{NH}_3)_6 + 2\text{Na}$	18.6
		$\text{Ca}(\text{NH}_3)_6\text{Na}_2 \rightarrow \text{Ca}(\text{NH}_3)_6 + \text{Na}_2$	2.8
		$\text{Ca}(\text{NH}_3)_6\text{Na}_2 \rightarrow \text{Ca} + 6\text{NH}_3 + 2\text{Na}$	81.8

## 2. Cartesian coordinates

Isomer **A** of  $\text{Mg}(\text{NH}_3)_6\text{Cl}_2$  at the CAM-B3LYP/6-311++G(d, p) level

N	-1.54085883	-0.88961526	1.35737015
N	-1.54085883	0.88961526	-1.35737015
N	1.54085883	-0.88961526	1.35737015
N	1.54085883	0.88961526	-1.35737015
N	-0.00000000	1.77923052	1.35737015
N	0.00000000	-1.77923052	-1.35737015
H	0.81113913	2.38898387	1.30258458
H	-0.81113913	2.38898387	1.30258458
H	-0.00000000	1.38656973	2.31659089
H	-1.20080461	0.69328487	-2.31659089
H	-2.47449028	0.49202485	-1.30258458
H	-1.66335116	1.89695903	-1.30258458
H	1.66335116	1.89695903	-1.30258458
H	2.47449028	0.49202485	-1.30258458
H	1.20080461	0.69328487	-2.31659089
H	0.00000000	-1.38656973	-2.31659089
H	0.81113913	-2.38898387	-1.30258458
H	-0.81113913	-2.38898387	-1.30258458
H	2.47449028	-0.49202485	1.30258458
H	1.20080461	-0.69328487	2.31659089
H	1.66335116	-1.89695903	1.30258458
H	-2.47449028	-0.49202485	1.30258458
H	-1.66335116	-1.89695903	1.30258458
H	-1.20080461	-0.69328487	2.31659089
Mg	0.00000000	0.00000000	0.00000000
Cl	0.00000000	0.00000000	-4.00562505
Cl	0.00000000	0.00000000	4.00562505

Isomer **B** of  $\text{Mg}(\text{NH}_3)_6\text{Cl}_2$  at the CAM-B3LYP/6-311++G(d, p) level

N	1.62656653	0.68659133	-1.54427449
N	-0.01024721	-1.49067944	-0.14189117
N	0.09772869	2.98214520	0.00953001
N	-1.62766126	0.71995994	1.52738774
N	1.56027687	0.62268514	1.58059046
N	-1.65353681	0.73607439	-1.52513383
H	1.23873959	0.21883609	2.45627601
H	2.25361910	-0.05529750	1.19978497
H	2.09128355	1.44939329	1.83960141
H	-0.83456700	-1.90681851	0.29677002
H	-0.05579009	-1.81113366	-1.10577811
H	0.85347833	-1.89747190	0.22624190
H	-2.27285644	-0.02318119	1.18446658

H	-1.35142421	0.44202539	2.46505211
H	-2.20951538	1.54493322	1.64509013
H	-2.27832132	-0.01606884	-1.16538284
H	-2.24859866	1.55448035	-1.62087594
H	-1.40362742	0.46601309	-2.47258828
H	-0.32308006	3.39068564	-0.82001453
H	-0.37705159	3.38471132	0.81231857
H	1.05793845	3.31197880	0.04252694
H	2.27584002	-0.03383864	-1.16381364
H	1.34977701	0.35279052	-2.46362007
H	2.19923859	1.50868807	-1.71410765
Mg	-0.00468292	0.69344129	-0.01093674
Cl	-3.30271814	-1.47210544	0.03303763
Cl	3.31090784	-1.46903909	0.03436426

Isomer C of  $\text{Mg}(\text{NH}_3)_6\text{Cl}_2$  at the CAM-B3LYP/6-311++G(d, p) level

N	-0.20101318	-2.21444765	1.08148034
N	1.65398631	-0.23231664	2.48741354
N	-1.46563441	0.04181468	-0.72257063
N	0.20101318	2.21444765	1.08148034
N	1.46563441	-0.04181468	-0.72257063
N	-1.65398631	0.23231664	2.48741354
H	2.47684396	-0.03644519	-0.62964053
H	1.22805227	-0.87296647	-1.28586766
H	1.22884812	0.77437871	-1.30564832
H	2.04399830	0.63195503	2.85025958
H	1.41398343	-0.81030719	3.28723895
H	2.40630624	-0.70891430	1.99750498
H	1.10140031	2.57721341	1.38296028
H	0.12239850	2.50189015	0.07569126
H	-0.49538286	2.76759392	1.57369001
H	-1.41398343	0.81030719	3.28723895
H	-2.40630624	0.70891430	1.99750498
H	-2.04399830	-0.63195503	2.85025958
H	-1.22805227	0.87296647	-1.28586766
H	-1.22884812	-0.77437871	-1.30564832
H	-2.47684396	0.03644519	-0.62964053
H	0.49538286	-2.76759392	1.57369001
H	-1.10140031	-2.57721341	1.38296028
H	-0.12239850	-2.50189015	0.07569126
Mg	-0.00000000	0.00000000	0.90487357
Cl	0.00000000	2.68333604	-1.95880545
Cl	-0.00000000	-2.68333604	-1.95880545

Isomer **A'** of Mg(NH<sub>3</sub>)<sub>6</sub>NaCl at the CAM-B3LYP/6-311++G(d, p) level

N	-1.54070689	-0.88952753	1.22741709
N	-1.54346286	0.89111870	-1.48541563
N	1.54070689	-0.88952753	1.22741709
N	1.54346286	0.89111870	-1.48541563
N	0.00000000	1.77905507	1.22741709
N	-0.00000000	-1.78223739	-1.48541563
H	-0.81100300	2.38905218	1.16854545
H	0.00000000	1.39033472	2.18844063
H	0.81100300	2.38905218	1.16854545
H	-1.24301244	0.71765357	-2.45761366
H	-2.47878544	0.49080671	-1.42245631
H	-1.66444380	1.90128780	-1.42245631
H	1.24301244	0.71765357	-2.45761366
H	1.66444380	1.90128780	-1.42245631
H	2.47878544	0.49080671	-1.42245631
H	-0.00000000	-1.43530714	-2.45761366
H	0.81434164	-2.39209452	-1.42245631
H	-0.81434164	-2.39209452	-1.42245631
H	2.47448138	-0.49217689	1.16854545
H	1.20406519	-0.69516736	2.18844063
H	1.66347838	-1.89687529	1.16854545
H	-2.47448138	-0.49217689	1.16854545
H	-1.66347838	-1.89687529	1.16854545
H	-1.20406519	-0.69516736	2.18844063
Mg	0.00000000	0.00000000	-0.12144647
Na	0.00000000	0.00000000	-5.15288893
Cl	0.00000000	0.00000000	3.87576997

Isomer **B'** of Mg(NH<sub>3</sub>)<sub>6</sub>NaCl at the CAM-B3LYP/6-311++G(d, p) level

N	-0.60079850	-1.51285138	1.56862973
N	1.59957109	-0.04058958	0.00000000
N	-2.88352389	0.06163610	0.00000000
N	-0.60079850	1.72585352	-1.51350868
N	-0.60079850	-1.51285138	-1.56862973
N	-0.60079850	1.72585352	1.51350868
H	-0.21771992	-1.21296633	-2.46139735
H	0.06208749	-2.22380764	-1.20039323
H	-1.45657925	-2.01375092	-1.79117221
H	2.04353491	0.39710786	-0.80438519
H	2.04353491	0.39710786	0.80438519
H	1.86861298	-1.03642640	0.00000000
H	0.16579295	2.36571769	-1.24327318
H	-0.41806886	1.48003889	-2.48714483



H	-1.41634857	2.33986253	-1.53157617
H	0.16579295	2.36571769	1.24327318
H	-1.41634857	2.33986253	1.53157617
H	-0.41806886	1.48003889	2.48714483
H	-3.25629931	0.54285936	0.81479422
H	-3.25629931	0.54285936	-0.81479422
H	-3.28933609	-0.87076657	0.00000000
H	0.06208749	-2.22380764	1.20039323
H	-0.21771992	-1.21296633	2.46139735
H	-1.45657925	-2.01375092	1.79117221
Mg	-0.60015790	0.07404211	0.00000000
Cl	1.48771607	-3.30161714	0.00000000
Na	1.64806121	4.60606370	0.00000000

Isomer **C'** of Mg(NH<sub>3</sub>)<sub>6</sub>NaCl at the CAM-B3LYP/6-311++G(d, p) level

N	-2.78686703	-0.25637238	-1.52169830
N	0.29470055	0.35055509	-1.66030732
N	-2.75902046	-0.43155228	1.51419344
N	0.30312983	0.30355264	1.66666220
N	-1.51108435	2.21173421	0.06110575
N	-0.44620197	-2.12023400	-0.05509901
H	-0.58152384	2.66282091	0.04741596
H	-2.01869457	2.61242902	-0.73166883
H	-1.97347312	2.57196718	0.89981256
H	1.16048928	-0.16040348	-1.44413329
H	0.01623991	0.07338224	-2.60315123
H	0.57075632	1.33506687	-1.72663507
H	1.15394650	-0.23635414	1.46520837
H	0.61111449	1.28115829	1.71080882
H	0.01316003	0.06211164	2.61571693
H	0.58094654	-2.05562861	-0.04675425
H	-0.70247859	-2.69936923	0.74194090
H	-0.69058120	-2.65484295	-0.88636829
H	-2.38285875	-0.60145428	2.44759548
H	-3.38621599	0.36941094	1.60702333
H	-3.35049827	-1.23312665	1.29236164
H	-2.49942717	0.09741745	-2.43491889
H	-3.10233334	-1.21519879	-1.67265759
H	-3.61535591	0.28181216	-1.26286253
Mg	-1.13510469	0.01390464	0.00214856
Na	3.17349842	1.53626483	0.02961782
Cl	2.77923326	-1.05651473	-0.02378294

Isomer **D'** of Mg(NH<sub>3</sub>)<sub>6</sub>NaCl at the CAM-B3LYP/6-311++G(d, p) level

N	1.54383704	0.96861477	-3.23299076
N	-0.14899636	1.77972953	-0.59319114
N	0.06692648	-1.82130948	-3.23299076
N	-1.46679281	-1.01889940	-0.59319114
N	-1.61076352	0.85269471	-3.23299076
N	1.61578917	-0.76083014	-0.59319114
H	-2.53578379	0.65737618	-2.84613517
H	-1.53826983	1.86995104	-3.28836311
H	-1.62740667	0.51185728	-4.19553621
H	-0.09985674	1.41905698	0.37643280
H	0.59844883	2.47599265	-0.65871624
H	-1.02680187	2.30449352	-0.63803949
H	-1.17901102	-0.79600697	0.37643280
H	-2.44349695	-0.71972443	-0.65871624
H	-1.48234900	-2.04148326	-0.63803949
H	1.27886776	-0.62305001	0.37643280
H	1.84504811	-1.75626822	-0.65871624
H	2.50915087	-0.26301026	-0.63803949
H	-0.85029018	-2.26715627	-3.28836311
H	0.37042193	-1.66530416	-4.19553621
H	0.69858742	-2.52474127	-2.84613517
H	1.83719637	1.86736508	-2.84613517
H	2.38856002	0.39720523	-3.28836311
H	1.25698475	1.15344688	-4.19553621
Mg	0.00000000	0.00000000	-1.91456066
Na	0.00000000	0.00000000	3.42399633
Cl	0.00000000	0.00000000	5.84774473

Isomer A'' of  $\text{Mg}(\text{NH}_3)_6\text{Na}_2$  at the CAM-B3LYP/6-311++G(d, p) level

N	1.54275162	-0.89070806	1.35693084
N	0.00000000	1.78141612	1.35693084
N	0.00000000	-1.78141612	-1.35693084
N	-1.54275162	0.89070806	-1.35693084
N	1.54275162	0.89070806	-1.35693084
N	-1.54275162	-0.89070806	1.35693084
H	1.66405149	1.90067091	-1.29034227
H	2.47805503	0.49077541	-1.29034227
H	1.24587919	0.71930869	-2.33071352
H	-0.81400354	2.39144632	1.29034227
H	0.00000000	1.43861737	2.33071352
H	0.81400354	2.39144632	1.29034227
H	-1.66405149	1.90067091	-1.29034227
H	-1.24587919	0.71930869	-2.33071352
H	-2.47805503	0.49077541	-1.29034227

H	-2.47805503	-0.49077541	1.29034227
H	-1.66405149	-1.90067091	1.29034227
H	-1.24587919	-0.71930869	2.33071352
H	-0.00000000	-1.43861737	-2.33071352
H	0.81400354	-2.39144632	-1.29034227
H	-0.81400354	-2.39144632	-1.29034227
H	1.24587919	-0.71930869	2.33071352
H	1.66405149	-1.90067091	1.29034227
H	2.47805503	-0.49077541	1.29034227
Na	0.00000000	0.00000000	5.06203771
Na	-0.00000000	-0.00000000	-5.06203771
Mg	0.00000000	0.00000000	0.00000000

Isomer **B''** of  $\text{Mg}(\text{NH}_3)_6\text{Na}_2$  at the CAM-B3LYP/6-311++G(d, p) level

N	0.00000000	1.79216519	0.33187504
N	1.55206058	-0.89608260	0.33187504
N	-1.51876017	0.99017932	2.97358924
N	-0.09814036	-1.81037455	2.97358924
N	1.61690053	0.82019523	2.97358924
N	-1.55206058	-0.89608260	0.33187504
H	2.39610301	0.16405090	3.06881142
H	2.02115324	1.68817702	2.61310124
H	1.30439802	1.02855720	3.92552835
H	1.73700501	-1.89113116	0.48366222
H	1.25320504	-0.81322012	-0.64947092
H	2.46159209	-0.42981308	0.38197318
H	0.45142757	-2.59445856	2.61310124
H	0.23855765	-1.64392042	3.92552835
H	-1.05597926	-2.15711152	3.06881142
H	-1.60302509	-1.91689475	0.38197318
H	-2.50627014	-0.55872489	0.48366222
H	-1.33087180	-0.67869734	-0.64947092
H	-1.54295567	0.61536323	3.92552835
H	-1.34012375	1.99306063	3.06881142
H	-2.47258080	0.90628154	2.61310124
H	0.07766676	1.49191746	-0.64947092
H	-0.85856700	2.34670782	0.38197318
H	0.76926512	2.44985605	0.48366222
Na	0.00000000	0.00000000	-3.85590663
Na	0.00000000	0.00000000	-6.94240688
Mg	0.00000000	0.00000000	1.65799019

Isomer **a'** of  $\text{Ca}(\text{NH}_3)_6\text{NaCl}$  at the CAM-B3LYP/6-311++G(d, p) level

N	-0.34240395	-2.32435811	1.68062049
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N	1.84618837	1.46081443	0.00000000
N	-2.51060219	0.08276015	0.00000000
N	-0.34240395	1.01545741	-2.15507429
N	-0.34240395	-2.32435811	-1.68062049
N	-0.34240395	1.01545741	2.15507429
H	-0.41787461	-2.08499812	-2.66391770
H	0.61037575	-2.65532672	-1.51745316
H	-0.97573584	-3.09932413	-1.51397783
H	1.55788932	2.43791632	0.00000000
H	2.44429499	1.30493169	0.80719580
H	2.44429499	1.30493169	-0.80719580
H	-0.59628780	1.93786126	-1.77996594
H	0.47124897	1.16378603	-2.74901745
H	-1.10780518	0.75898485	-2.77485868
H	-0.59628780	1.93786126	1.77996594
H	-1.10780518	0.75898485	2.77485868
H	0.47124897	1.16378603	2.74901745
H	-2.59204513	1.10680305	0.00000000
H	-3.02761100	-0.24018718	-0.81517579
H	-3.02761100	-0.24018718	0.81517579
H	0.61037575	-2.65532672	1.51745316
H	-0.41787461	-2.08499812	2.66391770
H	-0.97573584	-3.09932413	1.51397783
Cl	2.37102341	-1.76036426	0.00000000
Na	-1.84940132	4.25501458	0.00000000
Ca	0.02535846	-0.35377774	0.00000000

Isomer **b'** of Ca(NH<sub>3</sub>)<sub>6</sub>NaCl at the CAM-B3LYP/6-311++G(d, p) level

Ca	0.00000000	0.00000000	0.07274861
N	1.72083849	0.99352656	1.64771585
N	-1.72083849	0.99352656	1.64771585
N	1.76673260	-1.02002354	-1.41974487
N	-1.76673260	-1.02002354	-1.41974487
N	0.00000000	2.04004708	-1.41974487
N	-0.00000000	-1.98705312	1.64771585
H	-0.81154412	2.65111442	-1.39398241
H	0.81154412	2.65111442	-1.39398241
H	0.00000000	1.58795993	-2.35067593
H	-2.65806868	0.59418148	1.62178508
H	-1.36554169	0.78839586	2.59366824
H	-1.84361059	2.00486426	1.62178508
H	-2.70170449	-0.62273939	-1.39398241
H	-1.37521363	-0.79397996	-2.35067593
H	-1.89016037	-2.02837503	-1.39398241

H	-0.81445809	-2.59904573	1.62178508
H	0.81445809	-2.59904573	1.62178508
H	-0.00000000	-1.57679172	2.59366824
H	1.37521363	-0.79397996	-2.35067593
H	2.70170449	-0.62273939	-1.39398241
H	1.89016037	-2.02837503	-1.39398241
H	1.36554169	0.78839586	2.59366824
H	2.65806868	0.59418148	1.62178508
H	1.84361059	2.00486426	1.62178508
Na	0.00000000	0.00000000	5.25538735
Cl	0.00000000	0.00000000	-3.89102449

Isomer **c'** of Ca(NH<sub>3</sub>)<sub>6</sub>NaCl at the CAM-B3LYP/6-311++G(d, p) level

Ca	0.00000000	0.00000000	0.00000000
N	0.00000000	0.00000000	2.61134966
N	1.38478122	0.00000000	-2.16877701
N	-1.10327149	-2.30810872	0.19376361
N	-1.70618699	0.04942890	-1.93581102
N	2.21874086	-1.22735185	0.62445456
N	-1.77180244	1.74614298	0.65796167
H	2.70939697	-0.34384179	0.77300498
H	2.35826335	-1.79642112	1.45387808
H	2.68082626	-1.70394804	-0.14461216
H	0.99713821	0.80777274	-2.67305090
H	2.36017892	0.24401231	-1.99742449
H	1.37956003	-0.77547533	-2.83267652
H	-1.57805124	-0.58840250	-2.72347500
H	-2.70363322	0.03424124	-1.71550992
H	-1.52130562	0.99254423	-2.31194084
H	-1.79614879	2.35294912	-0.17164645
H	-2.74316263	1.50511154	0.85924515
H	-1.44819874	2.35071140	1.41299944
H	-0.98436916	-2.82089846	-0.67769766
H	-0.76376275	-2.90649099	0.94252357
H	-2.10676091	-2.20001946	0.32741056
H	0.61505026	0.81469834	2.64850441
H	-0.87992131	0.26576829	3.04405761
H	0.41318977	-0.72045515	3.19570257
Na	0.66459168	3.58800255	-1.47425238
Cl	1.70898671	2.08219727	0.62218180

Isomer **d'** of Ca(NH<sub>3</sub>)<sub>6</sub>NaCl at the CAM-B3LYP/6-311++G(d, p) level

Ca	-0.57677700	-0.00358900	-0.01218700
N	-1.11469900	2.48505500	-0.45978400

N	0.44581900	0.33275300	2.33890300
N	-2.57197900	-0.53521000	-1.59199000
N	-0.41429800	-2.45595300	0.64739800
N	-2.64182400	0.03512700	1.57306000
N	0.48515800	-0.99600800	-2.15744500
H	-2.42368800	0.60349700	2.38823000
H	-3.55004500	0.34068600	1.23244800
H	-2.75968700	-0.91885300	1.91081700
H	1.14331900	-0.42029800	2.36130100
H	0.98996300	1.19300400	2.27619400
H	-0.00753300	0.31745000	3.25131200
H	-0.75279000	-2.75276400	1.56562000
H	-0.74523200	-3.15899400	-0.01791500
H	0.61192600	-2.58360600	0.68745100
H	1.21645800	-1.59545100	-1.75744700
H	0.04249800	-1.55130200	-2.88824300
H	0.98870500	-0.23209000	-2.60755800
H	-3.47844800	-0.09682600	-1.44730000
H	-2.30099000	-0.34890500	-2.55496600
H	-2.71700200	-1.54175900	-1.52527200
H	-0.13436600	2.74467400	-0.58792600
H	-1.61892600	2.76655500	-1.29561900
H	-1.47802300	3.04438900	0.30685400
Na	3.35803700	-0.91598300	0.28421300
Cl	1.89728000	1.31046100	-0.39009200

Isomer e' of Ca(NH<sub>3</sub>)<sub>6</sub>NaCl at the CAM-B3LYP/6-311++G(d, p) level

Ca	0.00000000	0.00000000	1.78388528
N	0.00000000	2.03172961	0.31437318
N	1.75952946	-1.01586480	0.31437318
N	-1.85314903	0.93373354	3.26608836
N	0.11793755	-2.07174091	3.26608836
N	1.73521149	1.13800737	3.26608836
N	-1.75952946	-1.01586480	0.31437318
H	2.66469888	0.98805002	2.87183345
H	1.59253673	2.14825187	3.27687060
H	1.78554839	0.84155447	4.24050253
H	1.86468145	-2.03330262	0.33871667
H	1.41146379	-0.79885184	-0.63466693
H	2.70618862	-0.62970701	0.35271175
H	1.06417233	-2.45330320	3.27687060
H	-0.16396664	-1.96710750	4.24050253
H	-0.47667303	-2.80172194	2.87183345
H	-1.89843658	-2.02877458	0.35271175

H	-2.69323245	-0.59821019	0.33871667
H	-1.39755788	-0.82293758	-0.63466693
H	-1.62158174	1.12555302	4.24050253
H	-2.18802586	1.81367192	2.87183345
H	-2.65670906	0.30505133	3.27687060
H	-0.01390591	1.62178942	-0.63466693
H	-0.80775203	2.65848159	0.35271175
H	0.82855100	2.63151281	0.33871667
Na	0.00000000	0.00000000	-3.60469383
Cl	0.00000000	0.00000000	-6.03256883

Isomer **a''** of  $\text{Ca}(\text{NH}_3)_6\text{Na}_2$  at the CAM-B3LYP/6-311++G(d, p) level

Ca	0.00000000	-0.00000000	-0.00000000
N	1.73033502	-0.99900939	1.55581081
N	0.00000000	1.99801878	1.55581081
N	-0.00000000	-1.99801878	-1.55581081
N	-1.73033502	0.99900939	-1.55581081
N	1.73033502	0.99900939	-1.55581081
N	-1.73033502	-0.99900939	1.55581081
H	1.85306110	2.01025773	-1.52381733
H	2.66746481	0.59966912	-1.52381733
H	1.38062842	0.79710619	-2.50461510
H	-0.81440371	2.60992685	1.52381733
H	0.00000000	1.59421238	2.50461510
H	0.81440371	2.60992685	1.52381733
H	-1.85306110	2.01025773	-1.52381733
H	-1.38062842	0.79710619	-2.50461510
H	-2.66746481	0.59966912	-1.52381733
H	-2.66746481	-0.59966912	1.52381733
H	-1.85306110	-2.01025773	1.52381733
H	-1.38062842	-0.79710619	2.50461510
H	-0.00000000	-1.59421238	-2.50461510
H	0.81440371	-2.60992685	-1.52381733
H	-0.81440371	-2.60992685	-1.52381733
H	1.38062842	-0.79710619	2.50461510
H	1.85306110	-2.01025773	1.52381733
H	2.66746481	-0.59966912	1.52381733
Na	0.00000000	-0.00000000	5.17710355
Na	0.00000000	-0.00000000	-5.17710355

Isomer **b''** of  $\text{Ca}(\text{NH}_3)_6\text{Na}_2$  at the CAM-B3LYP/6-311++G(d, p) level

Ca	-0.00000000	-0.00000000	0.44005033
N	-1.75126466	1.58568081	1.39778550
N	-1.75126466	-1.58568081	1.39778550

N	1.75126466	1.58568081	1.39778550
N	0.00000000	-1.59877381	-1.52250877
N	0.00000000	1.59877381	-1.52250877
N	1.75126466	-1.58568081	1.39778550
H	-0.82750564	1.41039053	-2.09068681
H	0.00000000	2.60019781	-1.34262051
H	0.82750564	1.41039053	-2.09068681
H	-1.56998349	-2.58316028	1.30153655
H	-2.09184769	-1.44680852	2.34777481
H	-2.54893730	-1.38286952	0.78030142
H	-0.82750564	-1.41039053	-2.09068681
H	0.82750564	-1.41039053	-2.09068681
H	-0.00000000	-2.60019781	-1.34262051
H	2.54893730	-1.38286952	0.78030142
H	2.09184769	-1.44680852	2.34777481
H	1.56998349	-2.58316028	1.30153655
H	2.54893730	1.38286952	0.78030142
H	1.56998349	2.58316028	1.30153655
H	2.09184769	1.44680852	2.34777481
H	-2.09184769	1.44680852	2.34777481
H	-1.56998349	2.58316028	1.30153655
H	-2.54893730	1.38286952	0.78030142
Na	-4.20758256	0.00000000	-1.51337913
Na	4.20758256	-0.00000000	-1.51337913

Isomer c'' of Ca(NH<sub>3</sub>)<sub>6</sub>Na<sup>2</sup> at the CAM-B3LYP/6-311++G(d, p) level

Ca	0.00000000	0.00000000	1.55316367
N	0.00000000	2.01078856	0.03585938
N	1.74139397	-1.00539428	0.03585938
N	-1.74400269	1.06215493	3.05776519
N	-0.04785181	-2.04142810	3.05776519
N	1.79185450	0.97927317	3.05776519
N	-1.74139397	-1.00539428	0.03585938
H	2.68400107	0.49037702	2.95961923
H	1.97980651	1.96101884	2.84435319
H	1.55424311	0.94359599	4.05163398
H	1.86587011	-2.01636676	0.12509989
H	1.44269260	-0.84228162	-0.93444266
H	2.67457275	-0.59495598	0.11465847
H	0.70838888	-2.69507215	2.84435319
H	0.04005654	-1.81781201	4.05163398
H	-0.91732159	-2.56960162	2.95961923
H	-1.85253337	-2.01876996	0.11465847
H	-2.67915989	-0.60770753	0.12509989



H	-1.45078358	-0.82826763	-0.93444266
H	-1.59429965	0.87421602	4.05163398
H	-1.76667949	2.07922461	2.95961923
H	-2.68819539	0.73405331	2.84435319
H	0.00809098	1.67054925	-0.93444266
H	-0.82203938	2.61372594	0.11465847
H	0.81328978	2.62407429	0.12509989
Na	0.00000000	0.00000000	-4.06726326
Na	0.00000000	0.00000000	-7.16111451